

Sebacic acid, 3-chlorophenyl undecyl ester

Inchi: InChI=1S/C27H43ClO4/c1-2-3-4-5-6-7-10-13-16-22-31-26(29)20-14-11-8-9-12-15-21-27
InchiKey: VHCGASNROYVWCF-UHFFFAOYSA-N
Formula: C27H43ClO4
SMILES: CCCCCCCCCCOC(=O)CCCCCCCC(=O)Oc1cccc(Cl)c1
Mol. weight [g/mol]: 467.08

Physical Properties

Property code	Value	Unit	Source
gf	-200.53	kJ/mol	Joback Method
hf	-880.89	kJ/mol	Joback Method
hfus	69.11	kJ/mol	Joback Method
hvap	101.33	kJ/mol	Joback Method
log10ws	-9.29		Crippen Method
logp	8.440		Crippen Method
mvol	394.650	ml/mol	McGowan Method
pc	845.54	kPa	Joback Method
rinpol	3491.00		NIST Webbook
rinpol	3491.00		NIST Webbook
tb	1038.83	K	Joback Method
tc	1276.26	K	Joback Method
tf	607.23	K	Joback Method
vc	1.536	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1332.19	J/molxK	1038.83	Joback Method
cpg	1348.93	J/molxK	1078.40	Joback Method
cpg	1363.95	J/molxK	1117.97	Joback Method
cpg	1377.32	J/molxK	1157.54	Joback Method
cpg	1389.11	J/molxK	1197.12	Joback Method
cpg	1399.40	J/molxK	1236.69	Joback Method
cpg	1408.26	J/molxK	1276.26	Joback Method
dvisc	0.0002112	Paxs	607.23	Joback Method

dvisc	0.0001099	Paxs	679.16	Joback Method
dvisc	0.0000649	Paxs	751.10	Joback Method
dvisc	0.0000420	Paxs	823.03	Joback Method
dvisc	0.0000291	Paxs	894.96	Joback Method
dvisc	0.0000213	Paxs	966.90	Joback Method
dvisc	0.0000163	Paxs	1038.83	Joback Method

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U354867&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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